

**TURBULENCE IN THE STABLE PLANETARY BOUNDARY LAYER
AND ALOFT: MODELING AND CHARACTERIZATION USING DNS
AND LES**

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1. SUMMARY OF OBJECTIVES & PROGRESS

The objective of this project is to use a combined Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES) campaign to address the sub-grid-scale (SGS) parameterization of stratified turbulence and surface prescriptions. The work has three distinct components: conducting and analyzing the DNS solutions; conducting and analyzing the LES solutions; and improving the SGS description used in the LES so that LES predictive ability is enhanced.

During the last 12 months we have conducted focused analysis of our DNS solutions, explored new gravity-wave breaking simulations (including quantifying the turbulent Prandtl number), evaluated the numerics used in our LES code, conducted new work on optimal perturbation of stratified shear flows, extended verification comparisons between our DNS solutions and recent aircraft measurements (and found excellent agreement), and developed a Bayesian hierarchical methodology for deducing unresolved turbulent motions in mesoscale-model simulations of stratified flows. In addition, we also helped write a successful DoD High Performance Computing Modernization Program (HPCMP) proposal for challenge status for the computer work associated with this project and a successful DoD Golden Opportunity Capability Applications Projects (CAP) proposal that will provide an additional 1 to 2 million hours of computer time on newly delivered MPP systems before they are made generally available to DoD users. The CAP program benefits the DoD HPCMP by having new systems rigorously tested by experienced users.

This report focuses primarily on significant increase in performance of the new LES code we have developed for this project. We gauge the LES performance through comparison with our DNS. This has been the focus of our efforts during the last three months. For more detailed discussion of other achievements occurring earlier in the fiscal year, please refer to the quarterly reports covering that previous time period.

2. RECENT ACHIEVEMENTS

The most noteworthy achievement during the last three months is the significantly improved accuracy we have obtained with the LES code developed under this project for stably stratified shear turbulence. The code employs Germano's identity (Germano, et al., 1991, *Phys. Fluids*, 3, 1760-1765) with two filter widths (Δ and 2Δ) to implement a dynamic Smagorinsky SGS model for momentum flux and a similarly defined model for turbulent heat flux. Specifically, our model employs the following definition for the SGS vector heat flux q_i :

$$q_i = -C_q \Delta^2 |S| \frac{\partial T}{\partial x_i} \quad (1)$$

where C_q is the model coefficient, Δ is the filter width for resolved-scale features, $|S|$ is the resolved-scale strain rate, and $\partial T / \partial x_i$ is the resolved-scale temperature gradient. Equation (1) is also evaluated for results filtered by 2Δ ; this changes the values for q_i , $|S|$, and $\partial T / \partial x_i$, but it is assumed that C_q is independent of the filter width (this is the nature of Germano's identity). It is worth noting that the form used in Equation (1) is somewhat arbitrary. It is suggested by analogy with the Smagorinsky momentum-flux

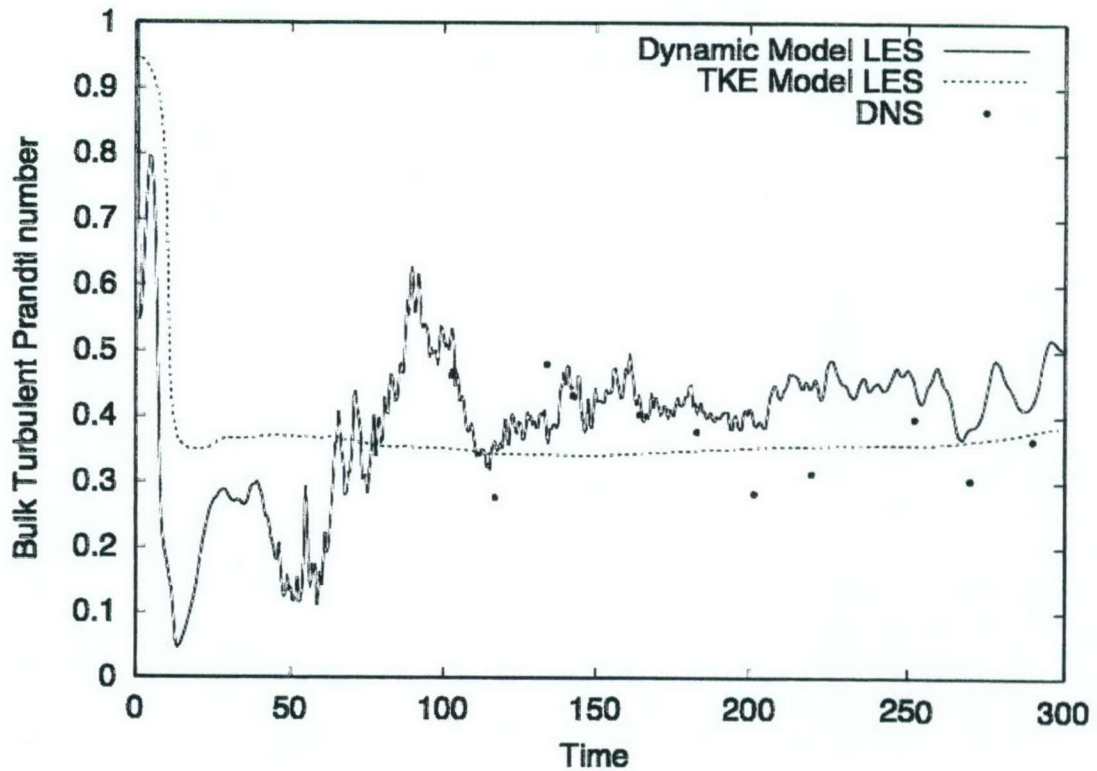


Figure 1. Turbulent Prandtl number versus time for TKE (dotted) and dynamic (solid) SGS procedures for $Re=2000$. Filtered DNS data are shown with solid symbols. The LES runs were conducted with a factor of 6 fewer grid points in each spatial direction and roughly 1300 times less computer time than the DNS, which was run with $720 \times 240 \times 1440$ spectral modes.

model, but it is by no means the only form one might select. Therefore, it should be understood that we employ Equation (1) as a first attempt, and we suggest a more complete analysis should be done to examine discrepancies that may result when using Equation (1). Nevertheless, as we demonstrate with Figures 1–3 below, results obtained with Equation (1) represent a significant improvement over the state-of-the-art TKE model with which we began this project.

The advantage to modeling the flux for both SGS momentum and heat, as we do here, is the resultant ability to compute the turbulent Prandtl number ($Pr_{turb} = \nu_e / \kappa_e$, where ν_e and κ_e are the eddy viscosity and eddy diffusivity) from the solution, rather than being forced to assume a value for it, as has typically been the case in work reported in the literature (and is also the case for our TKE model). We have employed both methods (and reported the results in our 26 Jan 2004 through 26 April 2004 quarterly report); however, our previous results suffered from an implementation bug, which we have since fixed. The new results are presented in Figure 1. The data points represent filtered DNS solutions. The solid (dotted) curves result from the dynamic (TKE) model. Pr_{turb} for the TKE model is a specified function of the local Richardson number. Its relatively good agreement with the DNS indicates the quality of the calibration used

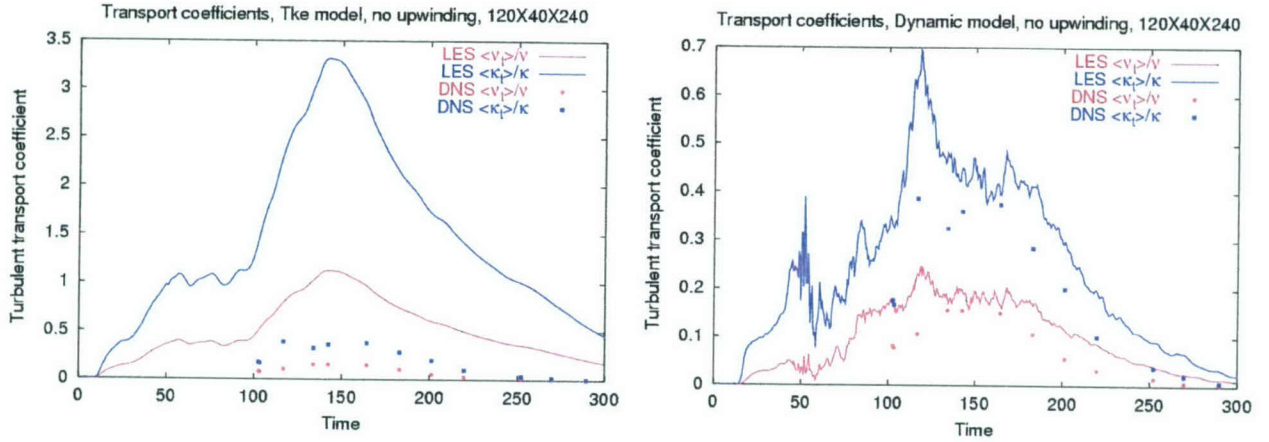


Figure 2. Eddy coefficients for momentum and heat for a) TKE and b) dynamic SGS models. ν_e (κ_e) is shown in red (blue). Data points indicate DNS results and are identical in both panels. Note the dramatic difference in the vertical scale required as the TKE results grossly over estimate the eddy coefficients.

to specify Pr_{turb} *a priori*. The results from the dynamic model are in excellent agreement, especially when one considers that they are in no way constrained, but instead result solely from Equation (1), the Smagorinsky model for SGS momentum, and the dynamic procedure.

Figure 1, by itself, would suggest the two procedures (TKE and dynamic modeling) are roughly equally accurate. However, when we examine ν_e and κ_e separately (as opposed to their ratio, Pr_{turb}) we see that the dynamic model is significantly more accurate than the TKE model. This is demonstrated in Figure 2, which shows the time histories of the eddy coefficients for the two procedures. Figure 2a shows the results from the TKE procedure. The eddy coefficients are grossly over predicted (by at least a factor of 5), indicating numerical solutions which are far too viscous and diffusive for the flow simulated. Figure 2b, which shows the results for the dynamic procedure, depicts a much more accurate solution, with the SGS quantities slightly *under* predicted (more is said about this result below – it is not a general result, and it indicates room for improvement).

In addition to the eddy coefficients, we have also examined the 2nd-order structure-function fits predicted by the LES models and compared them with DNS results. A plot including DNS results and those from the dynamic procedure is shown in Figure 3; it depicts profiles with height at 7 distinct times for the exponent α , coefficient C_T^2 , and inner scale ℓ_0 defined by fits to the 2nd-order structure function for temperature of the form $\Delta_r T^2 = C_T^2 r^\alpha$. The DNS results were previously validated against atmospheric measurements (see Werne & Fritts, 2000, DoD HPC User Group Conference proceedings, Albuquerque, NM and our 1 Feb 2004 through 30 April 2004 report.)

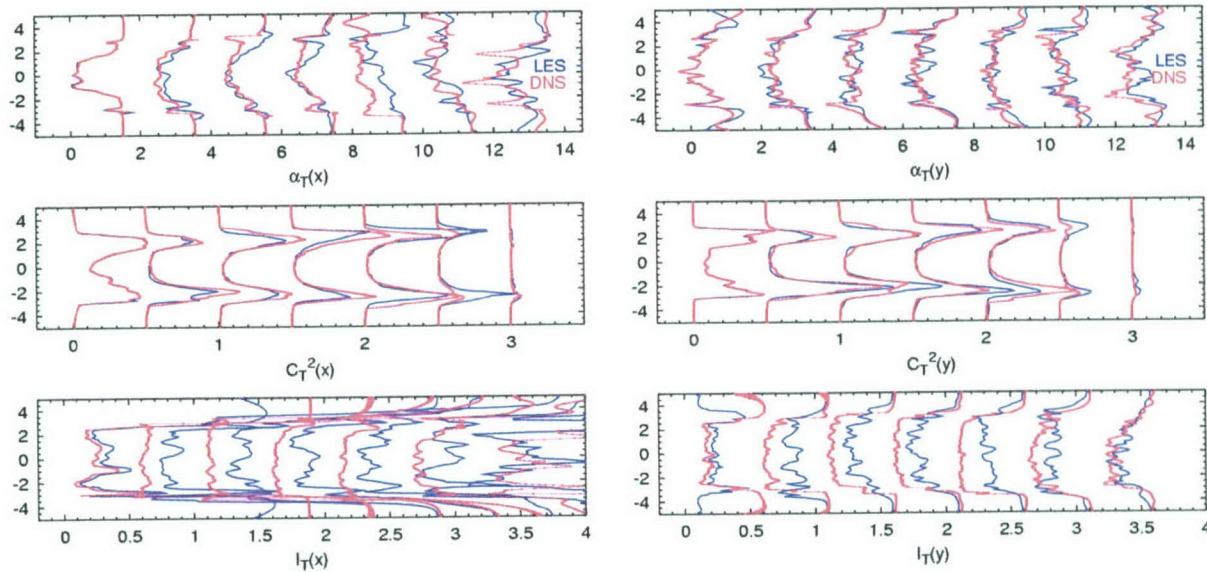


Figure 3. Structure-function-fit parameters versus height for LES (blue) and DNS (red) solutions. Structure functions are computed separately for streamwise (x) and spanwise (y) spatial separations. The two solutions are statistically indistinguishable, demonstrating that the LES is able to reproduce the DNS results while using 1300 times less computer time. See Werne & Fritts 2000 for details on the computation of the 2nd-order structure-function-fit parameters.

The results of Figures 2 and 3 indicate that a factor-of-6 reduction in the number of spectral modes used in each spatial direction with the dynamic LES procedure can reproduce the DNS results. Since the time step scales inversely with the number of modes in a spatial direction, this is equivalent to a factor of $6^4 \approx 1300$ savings in computer time. Hence, this allows us to now conduct LES simulations that both 1) span greater regions of parameter space and 2) attack problems involving atmospheric dynamics and physics occurring on larger scales of time and motion than is possible with the DNS. The results also indicate that we can indeed realize our initial goal of bootstrapping our way to improved parameterization schemes by employing DNS, LES and meso-scale models, as we have begun here (see the program plan we laid out in our original proposal for this work).

When we initiated this work, we did not know exactly how we would extend results from DNS and LES scales all the way to the much larger scales associated with mesoscale models. Recently, however, we developed a Bayesian Hierarchical Modeling (BHM) approach to address this need (see our 1 Nov 2003 through 31 Jan 2004 quarterly report). The model constructs the statistical likelihood of mesoscale SGS quantities based on combined computed and empirically obtained probability distributions. Such a probabilistic approach is the *only* manner in which an SGS model may be built when the resolving ability of the (mesoscale) simulation is near or excludes the peak in the energy spectrum, which is the case for stratified turbulent motions in *any* mesoscale model (even high-resolution models; see our 1 Nov 2003 through 31 Jan 2004 report). The difficulty with such a BHM approach, however, is establishing meaningful confidence in the procedures used to construct the *likelihood* and so-called *a priori* probability distributions. Nevertheless, because we have validated our DNS against atmospheric

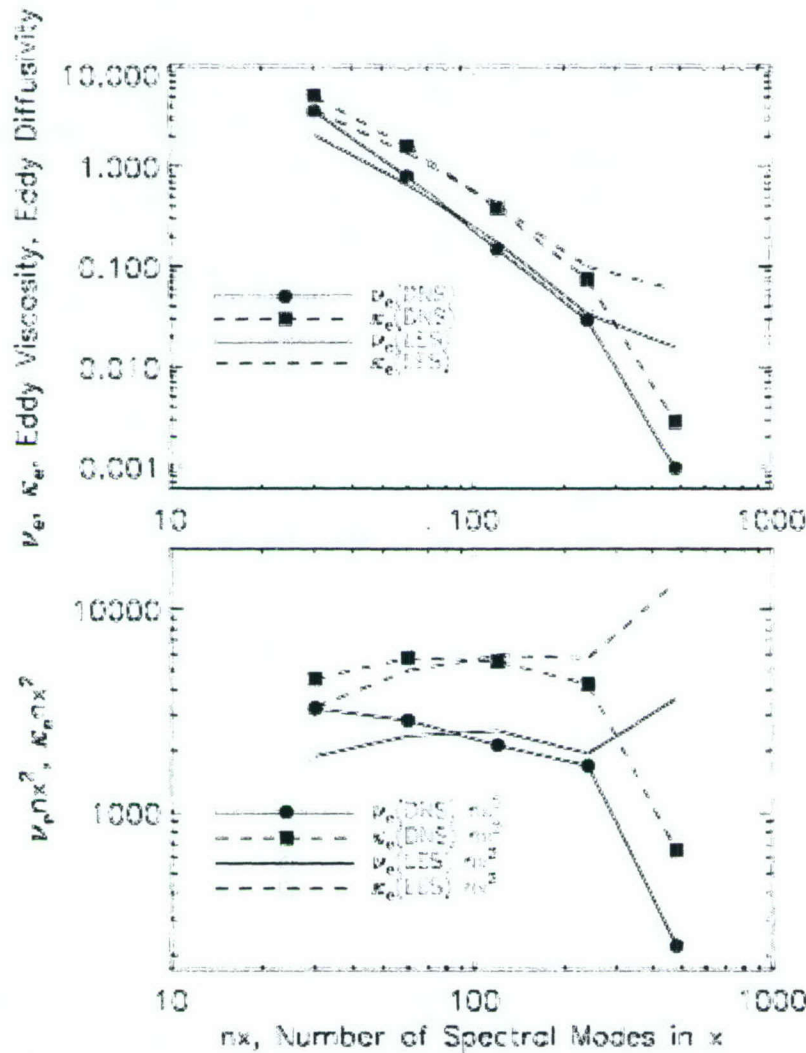


Figure 4. Eddy viscosity and eddy diffusivity for LES solutions (open symbols) versus numerical resolution. The original DNS results were computed with $720 \times 240 \times 1440$ spectral modes. D scales as $1/n_x$. LES results are compared with truncated DNS results (solid symbols). The lower panel shows compensated plots which are multiplied by n_x^2 (to remove the Δ^2 dependence of the eddy coefficients – see Equation 1). The remainder in the lower panel depends on the SGS strain rate S_{ij} . Note the different systematic dependences of the eddy coefficients for LES and DNS solutions. These differences between DNS and LES are understandable and acceptable at large values of n_x , as the SGS procedure is not designed to work in the dissipation range. However, the diverging results at low n_x is of concern and warrants further study. See text for additional discussion of this point and our plans for rectifying this situation.

observations and then our LES against our DNS (see Figures 2 and 3), we can have absolute confidence in the probability distributions we construct for the subgrid-scale $\langle u_i u_j \rangle$ and $\langle u_i \theta \rangle$ momentum and heat fluxes for stratified wind-shear events. We must now continue our program for wave-breaking and for coupling processes (likely mitigated by waves) between separate atmospheric mixing layers. However, with further refinement to our LES code, such work can be more complete, can be carried out on much larger domains (allowing for much better quantification of the needed *a priori*

probability distributions), and will proceed at a faster pace than the initial DNS studies conducted so far.

Nonetheless, in order to realize the goal of accurate and reliable SGS procedures for stratified turbulence at mesoscales which account for all relevant SGS processes, we must have confidence that the statistics derived from cataloged LES solutions are realistic for each of the phenomenon studied. Currently we have achieved this for wind shear. In order to obtain similarly validated results for wave breaking and for coupling between mixing layers, we must either: 1) obtain DNS solutions for these other problems or we must 2) demonstrate that the LES solution procedure we have implemented does not depend on the phenomenon studied or the filter scale Δ . Unfortunately, our solutions exhibit slight but noteworthy systematic dependence on Δ ; see Figure 4. Hence, before we can make further progress on a general SGS formulation for stratified dynamics, we must first improve our dynamic SGS scheme so that the Δ -dependence is removed. Currently we anticipate two potentially promising approaches for improvement. One involves examination of additional terms to augment Equation (1). The other involves extending the dynamic procedure to include a third filter width (at 3Δ perhaps) so that we may evaluate differences in the spectral slope at the different filter scales so that we are not forced to assume scale similarity at the cut-off and test-filter widths (as we do now). We will explore these alternate approaches if funding permits.

We have continued with the wave-breaking solutions begun earlier. We now have a sufficient number of runs to serve as a database against which new LES results can be compared.

3. PERSONNEL

The graduate student Matt Tearle, who was working on optimal perturbation problems related to this work, has obtained his Ph.D. and is no longer working on this project. To conserve resources, Dr. Joe Werne charged no time. Dr. Tom Lund charged only 56 hours total to this project during this reporting period.

4. TRAVEL

During the last three months, Dr. Tom Lund traveled to Williamsburg, VA in June to attend the annual DoD HPCMP User Group Meeting.

5. DIFFICULTIES

During the most recent three months of this reporting period we have throttled back our efforts significantly in order to conserve the limited funds that remain for use later in the year. At this point in the project, available funding is significantly below that anticipated by the original contract, so we are forced to reduce the work we do and concentrate on those items we feel are the most important. This is becoming especially frustrating now that our dynamic SGS model is performing well enough to allow us to perform much more realistic and informative parameter studies than we have been able to before. This is exacerbated by the knowledge that we have succeeded in securing possibly as much as two million more hours of supercomputer time through the HPCMO's new Golden Opportunity Capability Applications Projects (CAP) program, to which we applied during

this reporting period. The CAP computer time is in addition to the HPCMO Challenge Award we won with others. It represents a significant increase in resources for this project, but it also requires significant effort to port the code to the new IBM platform, conduct scalability tests, and complete a series of very large (i.e., 1000+ PE's) supercomputer runs.

6. PLANS

We plan to complete three journal articles currently in preparation, participate in the HPCMO CAP program (porting, testing, and running our Boussinesq code on the new IBM system (kraken) at NAVO), and complete analysis on new higher-Re gravity-wave simulations we have conducted. We hope we will be able to expand our parameter-space studies with the new stable-layer LES code we have developed, but that seems unlikely without additional funding. The new LES code represents the most promising development in this work to date. Combined with the new Bayesian approach we developed as part of this project for meso-scale model parameterization, results from new LES series could have a dramatic impact on the accuracy and reliability of SGS methods for Atmospheric Decision Aid modeling.